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On the Adiabatic Theorem in Quantum Theory

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PART II.

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Part II

Degenerate Adiabatic Transition

In the first part of this report a general treatment of the adiabatic theorem in quantum theory was given. It was shown that this theorem could be derived from an asymptotic expansion of the solution of the Schrödinger equation. This expansion proceeds in close analogy with the expansion of a solution of an ordinary differential equation.

The Schrödinger equation considered is the equation

$$i \nabla_t T = H(t,\tau)T$$

for a unitary operator T which reduces to the identity for $t = t_o$. The Hamiltonian H depends on the time t and, in addition, on a slowness parameter τ, see Part I, Section 1. The initial time t_o and the end time t_1 are to depend on the parameter τ in such a way that $t_1 - t_o \longrightarrow \infty$ as $\tau \longrightarrow \infty$.

This problem was treated in Part I under the assumption that the eigenvalues of the Hamiltonian H stay apart during the transition period $t_o \leqq t \leqq t_1$. The asymptotic expansion procedure that was used depends essentially on this assumption.

In the present report, Part II, we shall describe what

happens if this assumption is violated, specifically, if two eigenvalues of the Hamiltonian coalesce at some time during the process.

We speak of degenerate transition if at some time t during the transition process two eigenvalues of the Hamiltonian $H(t,\tau)$ coalesce. As was mentioned in the introduction to Part I, the adiabatic theorem remains valid in such a case, but the probability Pr_{non-ad} that the transition is not adiabatic may be of an order $> O(\tau^{-2})$ in the transition time $t_1 - t_o = \tau$, whereas it is of the order $O(\tau^{-2})$ if the transition is not adiabatic. The estimate $Pr_{non-ad} \leq O(\tau^{-1})$ was already given by Born and Fock in 1926.

Our aim is to describe the situation more precisely.

In order to determine the leading term of the asymptotic expansion of the solution T we can no longer rely on standard methods. A close analysis shows that the degeneracy corresponds exactly to the occurrence of a "turning point" in the terminology of the asymptotic theory of ordinary differential equations. The turning point encountered here is of a type which is somewhat different than that customarily treated; in fact, it is of a somewhat simpler type. It is not difficult to obtain the formulas for the transition across such a turning point.

As a result, among others, we obtain the leading term in the expansion of the probability Pr_{non-ad} with respect to τ,

and show that in general this term is actually of the order $O(\ ^{-1})$.

It is possible to give a simple description of the character of this leading term of Pr_{non-ad}. Consider the two eigenvectors--or principal axes--of the Hamiltonian whose eigenvalues will coalesce at some time. Denote by ϕ the angle these principal axes make with a reference position--a more precise definition of ϕ will be given at the end of this section--and by $\triangle E$ the difference of the two eigenvalues of the Hamiltonian. *The leading term of* Pr_{non-ad} *is then given by the simple formula*

$$(1) \qquad Pr_{non-ad} \sim 2\pi \frac{d\phi}{dt} \frac{d\phi}{d\triangle E} = 2\pi \left(\frac{d\phi}{dt}\right)^2 \Big/ \frac{d\triangle E}{dt} ,$$

in which the derivatives are to be evaluated at the time at which the two eigenvalues coalesce. Since $d\phi/dt$ is of the order $O(\tau^{-1})$ the same is true of Pr_{non-ad} if its "leading term", the right member of (1), does not vanish. We observe that this term does vanish if, at the time of coalescence, the rotating principal axes are instantaneously at rest relative to each other.

On the other hand we see that *the transition differs noticeably from an adiabatic one if the principal axes rotate fast relative to each other, while the difference* $\triangle E$ *of the two eigenvalues varies relatively slowly*.

We confine ourselves to the case in which *the Hilbert space of states is two-dimensional*. It may be assumed that the results are typical. Accordingly, the state $\underline{\Phi}$ may be given as a column ψ of two components ψ_1, ψ_2

$$\psi = \{\psi_1, \psi_2\} \tag{2}$$

and the Hamiltonian as a complex valued two-by-two matrix

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{22} & H_{22} \end{pmatrix} .$$

We assume that the matrix H depends on the time t and a parameter τ,

$$H = H(t,\tau), \quad \text{for } t_a \leq t \leq t_b \quad \text{and} \quad \tau > 0, \tag{4}$$

in such way that

$$H(t_a,\tau) = H_a, \quad H(t_b,\gamma) = H_b, \tag{5}$$

where the matrices H_a and H_b are given, independently of t_a, t_b and τ. We further assume that the times t_a and t_b depend on each other in such a way that

$$\tau = t_b - t_a . \tag{6}$$

We here deviate from our previous notation of denoting the initial time by $t = 0$ primarily because we want to reserve the value $t = 0$ for the time at which the two eigenvalues of $H(t,\tau)$ coalesce.

Our problem now is to describe asymptotically in the particular solution $T(t,\tau) = {}_aT(t,\tau)$ of the Schrödinger

equation

(7) $$i\nabla_t T(t,\tau) = H(t,\tau)T(t,\tau),$$

which reduces to the identity for $t = t_a$

(8) $${}_aT(t_a,\tau) = 1.$$

We assume that the matrix $H(T,\tau)$ is given as

(9) $$H(t,\tau) = H_{t/\tau}$$

in terms of a matrix H_s which depends analytically on a variable s in the neighborhood of the interval

(10) $$a \leq s \leq b.$$

Initial and end time are then given by

(11) $$t_a = \tau a, \quad t_b = \tau b.$$

In terms of the variable s we write the Schrödinger equation in the form

(12) $$i\nabla_s \psi_s = \tau H_s \psi_s$$

without imposing an initial condition for $s = a$. If $\psi_s = \psi_s(\tau)$ is a solution which possesses an inverse we obtain the Schrödinger matrix

(13) $$T(t,\tau) = T_{t/\tau}(\tau)$$

from the relation

(14) $${}_aT_s(\tau) = \psi_s(\tau)\ \psi_a^{-1}(\tau).$$

In particular we are interested in the matrix

$$(14)_b \qquad {}_aT_b(\tau) = \psi_b(\tau)\,\psi_a^{-1}(\tau),$$

which describes the transition from the initial time t_a to the end time t_b.

Equation (12) is nothing but a system of two ordinary differential equations of the second order. The theory of asymptotic expansions of solutions of such equations has been completely developed in the work of Horn, Birkhoff, and others, provided the eigenvalues of the matrix H_s are distinct. In the present problem, however, we want to make the assumption that the two eigenvalues coalesce at a certain point.

Specifically, we want to require that the two eigenvalues h_s^+ and h_s^- of the matrix $\underline{h}_s$ coalesce at $s=0$,

$$(15) \qquad h_0^+ = h_0^- ,$$

and differ for $s \neq 0$. We assume* that the labels $\pm$ may be assigned to them in such a way that the functions h_s^- and h_s^+ are analytic even at $s=0$. We further assume

$$(16) \qquad \nabla_s h_0^+ \neq \nabla_s h_0^- .$$

The point $s=0$ is a "turning point" for equation (12) since the Stokes phenomenon occurs when this point is encircled in the s-plane. That means, the analytic character

---

[*] Actually, the existence of such analytic functions follow from the assumed analyticity of H_s by Rellich's theorem

of the asymptotic expansion of solutions changes upon crossing certain lines, "Stokes lines", issuing from this point.

Suppose one chooses a solution ψ_s with a known asymptotic expansion which is valid as $a \leq s < 0$. Then it is necessary to determine the asymptotic behavior of this function ψ_s in the interval $0 < s \leq b$ in order to be able to give an asymptotic description of the matrix ${}_aT_b = \psi_b \psi_a^{-1}$, cf. $(14)_b$. In other words, it is necessary to solve the problem of "continuation" of the asymptotic expansion through the turning point.

To this end it is first necessary to introduce solutions ψ_s which have standard asymptotic expansions in appropriate neighborhoods of the point $s = 0$. To do this it is advisable to bring the matrix H_s into diagonal form.

Evidently, the Hermitian matrix H_s can be written in the form

$$H_s = \frac{1}{2}(h_s^+ + h_s^-)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{1}{2}(h_s^+ - h_s^-)\begin{pmatrix} \cos 2\phi_s & -e^{2i\eta_s}\sin 2\phi_s \\ -e^{-2i\eta_s}\sin 2\phi_s & -\cos 2\phi_s \end{pmatrix}$$

with appropriate real valued functions ϕ_s and η_s. We assume that functions ϕ_s and η_s exist which are analytic in s for $s_b \leq s \leq s_c$ such that (17) holds. With the aid of the unitary matrix

$$(18) \qquad U_s = \begin{pmatrix} e^{i\eta_s}\cos\phi_s & e^{i\eta_s}\sin\phi_s \\ -e^{-i\eta_s}\sin\phi_s & e^{-i\eta_s}\cos\phi_s \end{pmatrix},$$

and its adjoint and inverse

$$(18)^* \qquad U_s^* = \begin{pmatrix} e^{-i\eta_s}\cos\phi_s & -e^{-i\eta_s}\sin\phi_s \\ e^{i\eta_s}\sin\phi_s & e^{-i\eta_s}\cos\phi_s \end{pmatrix},$$

the matrix H_s can then be transformed into the diagonal matrix

$$(19) \qquad \Omega_s = \begin{pmatrix} h_s^+ & 0 \\ 0 & h_s^- \end{pmatrix} = U_s^* H_s U_s .$$

Since the matrix U_s here diagonalizes the matrix H_s, the role of the matrix U_s introduced in Section 2, which transformed H_s into H_o. The essential difference in the final formulas is that now not necessarily $U_a = 1$. Of course, we could achieve $U_a = 1$ by assuming H_a to be diagonal to being with.

From the discussions in Section 4 we know that the matrix KU_s, defined by (4.1) plays an important role. We find

$$(20) \qquad KU_s = iU_s^*\nabla_s U_s$$

$$= \nabla_s\phi_s \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \nabla_s\eta_s \begin{pmatrix} \cos 2\phi_s & -\sin 2\phi_s \\ -\sin 2\phi_s & -\cos 2\phi_s \end{pmatrix}.$$

In accordance with the theory of Section 7, U_s should be replaced by a matrix W_s for which KW_s has no diagonal terms. In order to eliminate the diagonal terms we introduce a real number ξ_s such that

(21) $$\nabla_s \xi_s = - \nabla_s \eta_s \cos 2\phi_s \, .$$

Then we set

(22) $$W_s = U_s \begin{pmatrix} \exp\left\{ i\xi_s \right\} & 0 \\ 0 & e\left\{ -i\xi_s \right\} \end{pmatrix} .$$

For their matrix W_s, evidently,

(23) $$K_s = KW_s = \begin{pmatrix} 0 & -i\nu_s^{+} \\ i\nu_s^{-} & 0 \end{pmatrix}$$

when we set

(24) $$\nu_s^{\pm} = [\nabla_s \phi_s \mp i \nabla_s \eta_s \sin 2\phi_s] \exp\left\{ \mp 2i\xi_s \right\} .$$

Obviously, the matrix H_s is transformed into the diagonal matrix

(25) $$\begin{pmatrix} h_s^{+} & 0 \\ 0 & h_s^{-} \end{pmatrix} = W_s^{*} H_s W^{s}$$

by W_s just as well as by U_s.

A few remarks may be made about the significance of the quantities $\nu_s^{\pm}$. While the quantities ϕ_s, $\nabla_s \phi_s$, and $\nabla \eta_s$ depend on the representation employed to represent the state

by a column of two numbers $\psi = \psi_1, \psi_2$, the quantities $\nu_s^{\pm}$ are independent of such a representation. For, if we change this representation by placing in front of U_s a unitary operator which is independent of s, the operator KU_s is not changed as seen from (20). The quantities $\nu_s^{\pm}$ are not changed if the diagonal representation is changed in such a way that the diagonal terms of K_s remain zero. For, such a change could be effected only by adding constants to the exponents ξ_s and $-\xi_s$ occurring in (22). As seen from (24) the expression $\nu_s^{\pm}$ would then receive only factors of absolute value 1. Furthermore, the absolute value

$$(24)' \qquad |\nu_s| = |\nu_s^{+}| = |\nu_s^{-}|.$$

To give the quantity $|\nu_s|$ a simple interpretation we may imagine that the original representation was so chosen that the Hamiltonian was diagonal for $s = 0$. Then $\phi_0 = 0$. Choosing further $\xi_0 = 0$, which we may do, we have $\nu_s^{\pm} = \nabla_s \phi$. We therefore feel justified in saying that $|\nu_s|$ is the angular speed with which the principal axes turn at the time at which the two eigenvalues coalesce.

For the purpose of asymptotic expansion we introduce the integrated eigenvalues

$$(26) \qquad \theta_s^{\pm} = \int_0^s h_\sigma^{\pm} d\sigma ,$$

and form the diagonal matrices

(27) $$\Theta_s = \begin{pmatrix} \theta_s^+ & 0 \\ 0 & \theta_s^- \end{pmatrix}$$

and

(28) $$\exp\left\{-i\tau\Theta_s\right\} = \begin{pmatrix} \exp\left\{-i\tau\theta_s^+\right\} & 0 \\ 0 & \exp\left\{-i\tau\theta_s^-\right\} \end{pmatrix} .$$

According to the theory of Horn

(29) $$\psi_s = W_s \chi_s \exp\left\{-i\tau\Theta_s\right\}$$

in which the matrix χ_s possesses an asymptotic power series expansion

(30) $$\chi \sim \sum_{\kappa=0}^{\infty} \tau^{-\kappa}\chi_s^{(\kappa)}$$

As this was done in Section 8 one could write down the differential equations to be satisfied by the χ_s and show that they can be solved successively. For the present purpose, however, it is more appropriate to write down the equations to be satisfied by the individual components.

We first introduce the columns composing the matrices ψ and χ.

(31) $$\psi = \overset{+}{\psi}, \overset{-}{\psi} , \qquad = \overset{+}{\chi}, \overset{-}{\chi}$$

and their components

(32) $$\overset{\pm}{\psi} = \overset{\pm}{\psi}_1, \overset{\pm}{\psi}_2, \quad \overset{\pm}{\chi} = \overset{\pm}{\chi}_1, \overset{\pm}{\chi}_2 ,$$

so that we may write

$$= \begin{pmatrix} \overset{+}{\psi}_1 & \overset{-}{\psi}_1 \\ \overset{+}{\psi}_2 & \overset{-}{\psi}_2 \end{pmatrix}, \quad \chi = \begin{pmatrix} \overset{+}{\chi}_1 & \overset{-}{\chi}_1 \\ \overset{+}{\chi}_2 & \overset{-}{\chi}_2 \end{pmatrix}$$

Here, and frequently in the following, we omit the subscript s. Relation (29) can now be written in the form

(34) $$\overset{\pm}{\psi} = W\overset{\pm}{\chi} \exp\left\{-i\theta^{\pm}\right\}.$$

From (12) we then obtain the equations

$(35)^+$ $$\begin{aligned} i\,\nabla_s \overset{+}{\chi}_1 &= i\nu^+ \overset{+}{\chi}_2 \\ i\,\nabla_s \overset{+}{\chi}_2 &= -\tau h \overset{+}{\chi}_2 - i\nu^- \overset{+}{\chi}_1 ; \end{aligned}$$

$(35)^-$ $$\begin{aligned} i\,\nabla_s \overset{-}{\chi}_1 &= \tau h \overset{-}{\chi}_1 + i\nu^+ \overset{-}{\chi}_2 , \\ i\,\nabla_s \overset{-}{\chi}_2 &= - i\nu^- \overset{-}{\chi}_1 , \end{aligned}$$

for the components of χ using the abbreviations

(36) $$h = h^+ - h^-$$

and the pair of complex conjugate numbers $\nu^{\pm}$ defined by (24).

We now insert the formal expansion (30). We first find that the leading term $\chi^{(o)}$ is to satisfy the condition

$$\overset{+}{\chi}{}^{(o)}_2 = \overset{-}{\chi}{}^{(o)}_1 = 0.$$

As solution we naturally choose

(36) $$\chi_s^{(o)} = 1$$

i.e.,

$$\begin{pmatrix} \overset{+}{\chi}{}_1^{(o)} & \overset{-}{\chi}{}_1^{(o)} \\ \overset{+}{\chi}{}_2^{(o)} & \overset{-}{\chi}{}_2^{(o)} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

For the terms of next order we find first

(37) $$\overset{+}{\chi}{}_2^{(1)} = i\frac{\nu^-}{h}, \quad \overset{-}{\chi}{}_2^{(1)} = i\frac{\nu^+}{h}$$

and then

(38) $$\overset{+}{\chi}{}_1^{(1)} = -i\int\frac{|\nu|^2}{h}\,ds, \quad \overset{-}{\chi}{}_2^{(1)} = i\int\frac{|\nu|^2}{h}\,ds\,.$$

Here we have used the abbreviation

$$|\nu|^2 = \nu^+\nu^-$$

which is justified since ν^+ and ν^- are complex conjugate by (24), cf. (24)'.

Formula (38) involves only a simple integration because the matrix W was so chosen that $K = KW$ had no diagonal terms, cf. (23). Using relations (36) to (38) we may write the matrix χ_s in 2nd approximation as

(39) $$\chi_s = \{\overset{+}{\chi}_s, \overset{-}{\chi}_s\} \sim \begin{pmatrix} 1 - \frac{i}{\tau}\int_{s_o}^{s}\frac{|\nu_\sigma|^2}{h_\sigma}\,d\sigma & \frac{i\nu_s^+}{\tau h_s} \\ \frac{i\nu_s^-}{\tau h_s} & 1 + \frac{i}{\tau}\int_{s_o}^{s}\frac{|\nu_\sigma|^2}{h_\sigma}\,d\sigma \end{pmatrix}$$

Since by (36), (15), and (16), the function h_s vanishes at $s = o$ the diagonal terms of the asymptotic approximation to χ_s have a logarithmic singularity at $s = 0$, although any solution χ_s itself is regular there.

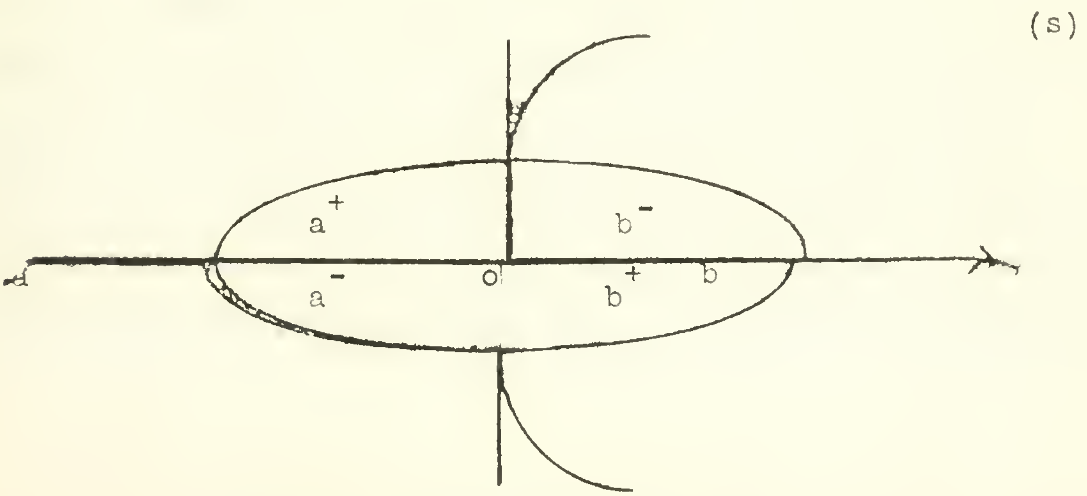
The theory of asymptotic expansion of solutions of ordinary differential equations enables us to assert the existence of solutions which possess asymptotic expansions are valid in certain regions to be described. These regions are separated by the arcs issuing from the turning point along which

(40) $$\operatorname{Im} \theta_s = 0,$$

where

(41) $$\theta_s = \theta_s^{+} - \theta_s^{-}.$$

The arcs will be called "transition lines". Since the eigenvalues $h_s^{\pm} = s\theta_s^{\pm}$ are real, the two rays of the real axis are such transition lines. Since θ_s vanishes at $s = 0$ of second order, there is another pair of transition lines, tangential to the imaginary axis.



Regions bounded by transition lines in the s-plane

The four transition lines divide a neighborhood of the segment $a \leq s \leq b$ into four open regions, denoted by $a^{\pm}$ and $b^{\pm}$ as indicated in the figure. Clearly $\operatorname{Im} \theta_s$ has the same sign in opposite regions. To fix the ideas we assume

$$
\begin{aligned}
(42) \qquad \operatorname{Im} \theta_s &> 0 \quad \text{in } b^- \text{ and } a^-, \\
&< 0 \quad \text{in } b^+ \text{ and } a^+.
\end{aligned}
$$

Consequently,

$$
(43) \qquad
\begin{aligned}
\exp\left\{i\tau\theta_s^+\right\} \exp\left\{-i\tau\theta_s^-\right\} &= \exp\left\{i\tau\theta_s\right\} \longrightarrow 0 \quad \text{in } b^- \text{ and } a^-, \\
\exp\left\{i\tau\theta_s^-\right\} \exp\left\{-i\tau\theta_s^+\right\} &= \exp\left\{-i\tau\theta_s\right\} \longrightarrow 0 \quad \text{in } b^+ \text{ and } a^+.
\end{aligned}
$$

With reference to the functions $\overset{\pm}{\psi}_s$, described by (34), we accordingly say that a function $\overset{+}{\psi}_s$ dominates a function $\overset{-}{\psi}$ in the regions b^- and a^-, while a function $\overset{-}{\psi}_s$ dominates a function $\overset{+}{\psi}_s$ in the regions b^+ and a^+. We shall also say that a function $\overset{-}{\psi}_s$ is "recessive" in regions b^- and a^- while a function $\overset{+}{\psi}_s$ is recessive in regions b^+ and a^+.

Now, according to the general theory, there does exist to each of the four sectors a solution which possesses an asymptotic expansion of one of the two types given by (34), in three adjacent sectors, the types being such that the solution is recessive in the inner sector and "dominant" in the two outer sectors. We denote there four "standard" solutions by ${}_a\overset{+}{\psi}_s$, ${}_a\overset{-}{\psi}_s$, ${}_b\overset{+}{\psi}_s$, ${}_b\overset{-}{\psi}_s$, so that they are recessive in the four sectors a^+, a^-, b^+ and b^- respectively. We may choose these solutions such that the asymptotic expansion of

the corresponding columns ${}_a\overset{\pm}{\chi}_s$, ${}_b\overset{\pm}{\chi}_s$, are given by (39) when the lower limit of integration in the diagonal terms is taken $s_o = a$ for ${}_a\overset{\pm}{\chi}_s$ and $s_o = b$ for ${}_b\overset{\pm}{\chi}_s$.

The problem of continuation now is the problem of finding an asymptotic description of each of the standard solutions in the respective "fourth" or "external" sector--including the "Stokes lines", i.e., the two transition lines bounding this sector. In fact, for our present purpose it would be sufficient to give an asymptotic description of each of these solutions on each of its Stokes lines.

In order to effect this continuation one need only express the solution as a linear combination of two other standard solutions. The known asymptotic expansion of these solutions then yields the asymptotic expansion of the first solution in its external sector and on its Stokes lines.

In particular, we may take the two solutions ${}_a\overset{\pm}{\psi}_s$ and express them in terms of the solutions ${}_b\overset{\pm}{\psi}_s$ with the aid of four coefficients $p^{\pm}_{\pm} = p^{\pm}_{\pm}(\tau)$.

$$
\begin{aligned}
{}_a\overset{+}{\psi}_s &= p^{+}_{+}\ {}_b\overset{+}{\psi}_s + p^{+}_{-}\ {}_b\overset{-}{\psi}_s, \\
{}_a\overset{-}{\psi}_s &= p^{-}_{+}\ {}_b\overset{+}{\psi}_s + p^{-}_{-}\ {}_b\overset{-}{\psi}_s .
\end{aligned}
\tag{44}
$$

Introducing the matrices ${}_a\psi = {}_a\overset{+}{\psi}, {}_a\overset{-}{\psi}$, ${}_b = {}_b\overset{+}{\psi}, {}_b\overset{-}{\psi}$ and the matrix

$$P = \begin{pmatrix} p_+^+ & p_+^- \\ p_-^+ & p_-^- \end{pmatrix} \tag{45}$$

we may write relations (44) in the form

$$ {}_a\psi = {}_b\psi P. \tag{46}$$

In order to determine the matrix P it is sufficient to determine the quotient of the matrices ${}_a\psi_s$ and ${}_b\psi_s$ at any suitable point s. It is natural to choose the turning point $s = 0$ itself for this purpose.

Note that at the origin ψ, agrees with W ,

$$\psi_o = W_o \chi_o ,$$

since the exponent θ_s vanishes for $s = o$. Hence we may determine the matrix P from the relation

$$P = {}_b\chi_o^{-1}\, {}_a\chi_o . \tag{47}$$

The function ${}_a\psi_s$ is given by its behavior at the point $s = a$ and that of the function ${}_b\psi_s$ is given by its behavior at the point $s = b$. Before we can determine the matrix P from (47) we must determine the matrices ${}_a\psi_s$ and ${}_b\psi_s$ at the point $s = o$. We may be satisfied with determining an asymptotic expansion of the matrix P. Accordingly, it is sufficient to determine the asymptotic expansion of the matrices ${}_a\psi_s = \left({}_a\overset{+}{\psi}_s,\ {}_a\overset{-}{\psi}_s\right)$ and ${}_b\psi_s = \left({}_b\overset{+}{\psi}_s,\ {}_b\overset{-}{\psi}_s\right)$ at the turning point $s = 0$.

The problem of deteмining the asymptotic expansions of the standard solutions ${}_a\psi_s$ and ${}_b\psi_s$ at the turning points will be referred to as the "connection" problem.

Note that the known asymptotic expansions of ${}_a\overset{\pm}{\psi}_s$ and ${}_b\overset{\pm}{\psi}_s$ are not valid at s = 0. In fact, some of the terms of these expansions are singular at s = 0. As seen from (38) the terms $\overset{+}{\chi}_1$ and $\overset{-}{\chi}_2$ have a logarithmic singularity at s = 0.

We shall describe a method* of handling the connection problem which seems to be particularly suitable if one is satisfied with determining only a few terms in the asymptotic expansion of ${}_a\psi_o$ and ${}_b\psi_o$; in fact, we shall be satisfied with only two terms.

The method, which we shall describe, will be referred to as the method of "stretching". In fact, the earlier treatments of the turning point problem employed more or less this method.

We shall introduce a new independent variable; instead of the variable s, viz., the variable

(48) $$a = [\tau \theta_s]^{1/2} .$$

Here θ_s was given by (41) and (26). For simplicity we shall assume

(49) $$\nabla_s h_s > 0,$$

---

* A different method, analogous to Langer's method of treating the turning point problem of an equation of the form $\omega'' = q\,\omega$ will be described elsewhere.

without restriction, so that $\theta_s \geq 0$.

The quantities $\overset{\pm}{\chi}_1$ and $\overset{\pm}{\chi}_2$ will now be considered a function of α. In view of

$$2\alpha d\alpha = \tau h_s ds,$$

$$(50)^+ \qquad \begin{aligned} i\nabla_\alpha \overset{+}{\chi}_1 &= \qquad\qquad - i\tau^{-1/2}\lambda^+\overset{+}{\chi}_2 \, , \\ i\nabla_\alpha \overset{+}{\chi}_2 &= -2\alpha\overset{+}{\chi}_2 + i\tau^{-1/2}\lambda^-\overset{+}{\chi}_1 \, ; \end{aligned}$$

$$(50)^- \qquad \begin{aligned} i\nabla_\alpha \overset{-}{\chi}_1 &= 2\alpha\overset{-}{\chi}_2 - i\tau^{-1/2}\lambda^+\overset{-}{\chi}_2 \, , \\ \nabla_\alpha \overset{-}{\chi}_2 &= \qquad\qquad i\tau^{-1/2}\lambda^-\overset{-}{\chi}_1 \, ; \end{aligned}$$

in which $\lambda^\pm = \lambda^\pm(\beta,\tau)$ stands for

$$(51) \qquad \lambda^\pm = 2\,\theta_s^{1/2}\,\nu_s^\pm / h_s \, .$$

Note that the right member here approaches a finite value $\lambda_o^\pm$ as $s \rightarrow 0$. For, by (36), (15), (16), (26), (41), we have

$$h_s = s\nabla_s h_o + \ldots, \quad \theta_s = \frac{1}{2}\, s^2\nabla_s h_o + \ldots,$$

where $\nabla_s h_o = (\nabla_s h_s)^{s=0}$, and hence

$$\lambda^\pm = (2/\nabla_s h_o)^{1/2}\nu_o^\pm .$$

It is furthermore seen that the functions $\overset{\pm}{\lambda}(\alpha,\tau)$ are regular in $\tau^{-1/2}$ at $\tau = \infty$. Consequently, each of the pair of (50) possesses a two parametric set of independent solutions which are regular in $\tau^{-1/2}$. The standard solutions ${}_a\overset{\pm}{\psi}$ and ${}_b\overset{\pm}{\psi}$, when considered functions of α and τ, will be among these solutions of equations (50), except for a factor which will depend on τ and will not be regular in $\tau^{-1/2}$ at $\tau = \infty$. In other words, we expect that the solutions $\overset{\pm}{\chi} = {}_a\overset{\pm}{\chi}$ or $\overset{\pm}{\chi} = {}_b\overset{\pm}{\chi}$ are of the form

$$\overset{\pm}{\chi} = \overset{\pm}{c}(\tau)\,{}^{o}\overset{\pm}{\chi}(\alpha,\tau) \tag{53}$$

in which the functions ${}^{o}\overset{\pm}{\chi}(\alpha,\tau)$ are solutions of equations (50) which possess convergent expansions of the forms

$${}^{o}\overset{\pm}{\chi}(\alpha,\tau) = \sum_{\mu=0}^{\infty} {}^{o}\overset{\pm}{\chi}{}^{(\mu)}(\alpha)\,\tau^{-\mu/2} .$$

The problem now is to identify the standard solutions ${}_a\overset{\pm}{\psi}$, ${}_b\overset{\pm}{\psi}$ with appropriate solutions of equations (50).

Before explaining how this is to be done we make the following observation. As seen from (48), point α corresponds to a point s which depends on τ and approaches $s = 0$ as $\tau \longrightarrow \infty$. Vice versa, a point s corresponds to a point α which depends on , and approaches $\alpha = \infty$ as $\tau \longrightarrow \infty$. Therefore, it may be expected that the asymptotic behaviors of the solutions $\overset{+}{\chi}$ when considered as functions of (α,τ) and (s,τ) are connected only inasmuch as the latter behavior as $s \longrightarrow 0$ whould match the former behavior as $\alpha \longrightarrow \infty$.

More specifically, suppose one re-introduces the variable s in the terms $\overset{\pm}{\chi}[\mu]_\alpha$ occurring in the series (53) and develops the resulting function $\overset{\pm}{\chi}(\tau^{1/2}\theta_s^{1/2})$ asymptotically with respect to . Suppose that one further develops the coefficient $c(\tau)$ occurring in (53) asymptotically in τ. Then the terms resulting from the series (53) which are now multiplied by the same power of τ should add up to the term in the asymptotic expansion of the function $\overset{\pm}{\chi}$ considered a function of s.

Before computing the terms ${}^{o}\overset{\pm}{\chi}{}^{(\mu)}$ occurring in the series (54) we describe the behavior of the functions ${}_a\overset{\pm}{\chi}_s$ and ${}_b\overset{\pm}{\chi}_s$ near s = 0. From (39), (15), and (16) we have

$$\begin{aligned}
\overset{+}{\chi}_1 &\sim 1 - \frac{i}{\tau}\left[\frac{\nu_o^+\nu_o^-}{\nabla_s h_o}\log s + k\right], \\
\overset{+}{\chi}_2 &\sim \frac{i}{\tau s}\,\frac{\nu_o^+}{\nabla_s h_o}, \\
\overset{-}{\chi}_1 &\sim \frac{i}{\tau s}\,\frac{\nu_o^-}{\nabla_s h_o}, \\
\overset{-}{\chi}_2 &\sim 1 + \frac{i}{\tau}\left[\frac{\nu_o^+\nu_o^-}{\nabla_s h_o}\log s + k\right],
\end{aligned} \tag{55}$$

the constant k depending on whether the front subscript is a or b.

Introducing α instead of s as independent variable we find from (55) the expressions

$$(56)^+ \qquad \overset{+}{\chi}_1 \sim 1 - \frac{i}{\tau}\left[\frac{1}{2}\,\frac{\nu_o^+\nu_o^-}{\nabla_s h_o}\log\tau + g(\alpha)\right]$$

$$\overset{+}{\chi}_2 \sim \frac{2i\lambda_o^+}{\tau^{1/2}\alpha}$$

$$\overset{-}{\chi}_1 \sim \frac{2i\lambda_o^-}{\tau^{1/2}\alpha}$$

$$(56)^- \qquad \overset{-}{\chi}_2 \sim 1 + \frac{i}{\tau}\left[\frac{\nu_o^+\nu_o^-}{\nabla_s h_o}\log\tau + g(\alpha)\right]$$

with an appropriate function $g(\alpha)$.

Without proof we anticipate that the terms of higher order in the expansion of χ_s, which begins with the term (39), does not contribute terms of lower order in $\tau^{-1/2}$ and α^{-1} than those shown in (56).

We proceed to compute the terms $\overset{o\pm}{\chi}$ occurring in the series (54). As seen from $(50)^+$ the function ${}^{o}\overset{+}{\chi}{}^{(o)}$ is a solution of the equation

$$i\,\nabla_\alpha\, \overset{o+}{\chi}{}_1^{(o)} = 0$$

$$i\,\nabla_\alpha\, \overset{o+}{\chi}{}_2^{(o)} = 2\alpha\, {}^{o}\chi_2^{(o)},$$

hence of the form

$$ {}^{o}\overset{+}{\chi}{}_1^{(o)} = \overset{+}{j}_1, \qquad {}^{o}\overset{+}{\chi}{}_2^{(o)} = \overset{+}{j}_2 \exp\left\{i\alpha^2\right\}.$$

We now determine the constants γ_1 and γ_2 such that these functions agree with the functions $(56)^+$ when α approaches infinity in the sectors in which the asymptotic expansion (39)

of $\overset{\pm}{\chi}$ is valid.

In the sectors a^+ and b^+, where Im $\alpha^2 = \tau \,\mathrm{Im}\, \theta < 0$ by (42), we have $\exp\left\{i\alpha^2\right\} \longrightarrow \infty$ as $\alpha \longrightarrow \infty$. Therefore we should get $\overset{+}{\gamma}_2 = 0$. Without restriction we may get $\overset{+}{\gamma}_1 = 1$.

Similarly we should set $\overset{-}{\gamma}_1 = 0$ and may set $\gamma_2 = 1$, i.e.,

(57) $$ {}^{o}\chi^{(o)}_{(\alpha)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . $$

Having done so, we should set

(58) $$ \overset{\pm}{c}(\infty) = 1 $$

so that the term of lowest order in (53), (54) agrees with the term of lowest order in (56).

The term of next order in the expansion $(54)^+$ is a solution of the equation

$$ i \nabla_\alpha {}^{o}\overset{+}{\chi}{}^{(1)}_{1} = -i\lambda^{+}_{o}\, {}^{o}\overset{+}{\chi}{}^{(o)}_{2} = 0 $$

$$ i \nabla_\alpha {}^{o}\overset{+}{\chi}{}^{(1)}_{2} + 2\alpha\, {}^{o}\overset{+}{\chi}{}^{(1)}_{2} = i\lambda_o\, {}^{-o}\overset{+}{\chi}{}^{(o)}_{1} = i\lambda^{-}_{o} . $$

Hence ${}^{o}\overset{+}{\chi}{}^{(1)}_{1}$ is constant. Since $\overset{+}{\chi}_1 - 1$ vanishes of higher order than $\tau^{-1/2}$ as $\tau \longrightarrow \infty$, as seen from $(56)^+$, we should set this constant equal to zero, i.e.,

$(59)^+_1$ $$ {}^{o}\overset{+}{\chi}{}^{(1)}_{1} = 0. $$

Except for an additive multiple of $\exp\{i\alpha^2\}$, which will be seen to be zero, the function ${}^{o}\overset{+}{\chi}{}_2^{(1)}$ is found to be

$$(59)_2^+ \qquad {}^{o}\overset{+}{\chi}{}_2^{(1)} = \lambda_o^- \int_{\upsilon^+\infty}^{\alpha} \exp\left\{i\alpha^2 - i\beta^2\right\} d\beta \, .$$

Here υ^+ is a unit vector bisecting the quadrant which corresponds to the sector a^+ or b^+. Thus, if the function in question is ${}_a\overset{+}{\chi}$ or ${}_b\overset{+}{\chi}$ respectively, we have

$$(60)^+ \qquad {}_a\upsilon^+ = -\exp\left\{-i\pi/4\right\}, \quad {}_b\upsilon^+ = \exp\left\{-i\pi/4\right\}.$$

With these values of υ^+ the integral can be carried out along a ray in the direction of $-\upsilon^+$ from $\upsilon^+\infty$, i.e., from ∞ in the direction of υ^+, to α for every point in the region formed by the three quadrants and the included transition rays. By integration by parts one finds

$${}^{o}\overset{+}{\chi}{}_2^{(1)} \sim 2i\lambda_o^- \alpha^{-1} \quad \text{for} \quad \alpha \sim \infty$$

provided α lies in the region just mentioned.

From this result combined with (58) we obtain for the function for the function $\overset{+}{\chi}_2 = c(\tau)\overset{+}{\chi}_2$ in the lowest order the approximation

$$\overset{+}{\chi}_2 \sim 2i\tau^{-1/2}\lambda_o^-\alpha^{-1}$$

in agreement with $(56)_2^+$. This agreement shows that we were justified in omitting a constant of integration from formula (57).

In a similar fashion we find

(59)$^-$ $${}^{o}\chi_1^{(1)} = -\lambda_o^{+} \int_{\upsilon^{-}\infty}^{\alpha} \exp\left\{i\beta^2 - i\alpha^2\right\} d\beta ,$$

$${}^{o}\overset{-}{\chi}{}_2^{(1)} = 0;$$

with

(60)$^-$ $${}_a\upsilon^{-} = -\exp\left\{i\pi/4\right\}, \quad {}_b\upsilon^{-} = \exp\left\{i\pi/4\right\} .$$

Since the series (54) involves only powers of $\tau^{-1/2}$, the terms in (56) involving log τ can be matched only by terms resulting from an expansion of the factor $\overset{\pm}{c}(\tau)$. Specifically, we find

(61) $$\overset{\pm}{c} = 1 \mp \frac{i|\nu_o|^2}{2\nabla_s h_o} \tau^{-1} \log \tau ,$$

as improvement of relation (57).

We are now in the position to determine the asymptotic expansion of the standard functions $\overset{\pm}{\chi}_s$ at the turning point s = 0. We first note down the relation

(62) $$\int_{\upsilon^{\pm}\infty}^{0} \exp\left\{\mp i\beta^2\right\} d\beta = -\tfrac{1}{2}\pi^{1/2}\upsilon^{\pm} .$$

By (53), the value of the matrix χ_s, cf. (33), is given by

(63) $$\chi_s^{(\tau)} = \overset{o}{\chi}(\alpha,\tau)\, c(\tau)$$

with

$$(64) \qquad {}^{o}\chi(a,\tau) = \begin{pmatrix} {}^{o}\overset{+}{\chi}_1(a,\tau) & {}^{o}\overset{-}{\chi}_1(a,\tau) \\ {}^{o}\overset{+}{\chi}_2(a,\tau) & {}^{o}\overset{-}{\chi}_2(a,\tau) \end{pmatrix}$$

and

$$(65) \qquad C(\tau) = \begin{pmatrix} \overset{+}{c}(\tau) & 0 \\ 0 & \overset{-}{c}(\tau) \end{pmatrix} .$$

From (57) and (59) we infer that $\overset{o}{\chi}(a)$ for $a = 0$ is approximately given by

$$(66) \qquad {}^{o}\chi(o) \sim \begin{pmatrix} 1 & \frac{1}{2}\,(\pi/\tau)^{1/2}\lambda_o^{+}\upsilon^{-} \\ -\frac{1}{2}\,(\pi/\tau)^{1/2}\lambda_o^{-}\upsilon^{+} & 1 \end{pmatrix}$$

while $\overset{\pm}{c}(\tau)$ is given by (61).

From relation (47) we therefore may determine the transition matrix P as

$$P = C^{-1}\, {}^{o}_{a}\chi(o)^{-1}\, {}^{o}_{b}\chi(o)$$

$$\sim C^{-1} \begin{pmatrix} 1 & \frac{1}{2}\,(\pi/\tau)^{1/2}\lambda_o^{+}({}_b\upsilon^{-} - {}_a\upsilon^{-}) \\ \frac{1}{2}\,(\pi/\tau)^{1/2}\lambda_o^{-}({}_b\upsilon^{+} - {}_a\upsilon^{+}) & 1 \end{pmatrix}$$

or, since C = 1 in lowest order, by

$$(66) \qquad P \sim \begin{pmatrix} 1 & (\pi/\tau)^{1/2}\lambda_o^{+}\,\exp\{i\pi/4\} \\ -(\pi/\tau)^{1/2}\lambda_o^{-}\,\exp\{-i\pi/4\} & 1 \end{pmatrix} .$$

Thus the transition matrix is determined in first or second order.

We are now ready to describe asymptotically the Schrödinger operator

$$T_b = \psi_b \psi_a^{-1} ,$$

cf. $(14)_b$. As matrices ψ_s we chose ${}_a\psi_s$ so that ${}_aT_b$ is expressed as

$${}_aT_b = {}_a\psi_b \, {}_a\psi_a^{-1} ;$$

using (46) we may write

$$(67) \qquad {}_aT_b = {}_b\psi_b \, P \, {}_a\psi_a^{-1} .$$

Now we make use of (29) and write

$$(68) \qquad {}_aT_b = W_b \, {}_b\chi_b \exp\{-i\tau\Theta_b\} \, P \exp\{i\tau\Theta_a\} \, {}_a\chi_a^{-1} \, W_a^{-1} .$$

From the asymptotic description (39) of ${}_a\chi_s$ and ${}_b\chi_s$, with $s_o = a$ and $s_o = b$ respectively, we infer that the matrices ${}_a\chi_a$ and ${}_b\chi_b$ differ from the identity by terms of the order (τ^{-1}). Since the terms of second order in P are of order $(\tau^{-1/2})$ we replace ${}_a\chi_a$ and ${}_b\chi_b$ by 1 in formula (68). By (66) and (28) the result is

$$(69) \quad T_b \sim W_b \begin{pmatrix} \exp\{i\tau(\theta_a^+ - \theta_b^+) & (\pi/\tau)^{1/2} \lambda_o^+ \exp\{i\tau(\theta_a^- - \theta_b^+) + i\pi/4\} \\ -(\pi\tau)^{1/2} \lambda_o^- \exp\{i\tau(\theta_a - \theta_b) - i\pi/4\} & \exp i\tau(\theta_a^- - \theta_b^-)\} \end{pmatrix} W_a^{-1} .$$

The term of lowest order,

$$(70) \qquad T_b \sim W_b \exp\{i\tau(\Theta_a - \Theta_b)\} W_a^{-1}$$

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yields the adiabatic theorem in accordance with the explanations given in Section 3. In fact, in terms of the columns

$$(71) \qquad j^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad j^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

the eigen-states of the initial Hamiltonian H_o are given by multiples of $W_a j^\pm$; those of the end Hamiltonians by multiples of $W_b j^\pm$. The state $T_b W_a j^\pm$ into which the initial eigen-state $W_a j^\pm$ goes over during the process considered is given by (70) as

$$(72) \qquad T_b W_a j^\pm = \exp\left\{ i\tau(\theta_a^\pm - \theta_b^\pm)\right\} W_b j$$

and is thus seen to be an eigen-state of the end Hamiltonian.

If the improved formula (69) is used one finds that the initial eigen-state $W_a j^\pm$ goes over into the state

$$(72) \quad T_b W_a j^\pm = \exp\left\{ i\tau(\theta_a^\pm - \theta_b^\pm)\right\} W_b j^\pm$$
$$\mp (\pi/\tau)^{1/2} \lambda_o^\mp \exp\left\{ i\tau(\theta_a^\pm - \theta_b^\mp) \mp i\pi/4\right\} W_b j^\mp .$$

According to the principles of quantum theory, the absolute square of the coefficient of $W_b j^\mp$ gives the probability that the eigen-state $W_b j^\mp$. It is seen that this probabil- is independent of whether we begin with $W_a j^+$ or with $W_a j^-$. We are therefore, justified in referring to this probability as the probability of non-adiabatic transition. Thus we have

$$(73) \qquad Pr_{\text{non-ad}} = \pi\tau^{-1} |\lambda_o|^2$$

or, by (52)

$$\text{(75)} \qquad \mathrm{Pr}_{\text{non-ad}} = \frac{2\pi}{\tau|\nabla_s h_o|} |\nu_o|^2 .$$

We recall that $h_s = h_s^+ - h_s^-$ is the difference of the two eigenvalues of the Hamiltonian. The meaning of the term $|\nu_o| = |\nu_o^+| \tau |\nu_o^-|$ is given by (24). As was explained in connection with formula (24)' the expression ν_o may be interpreted as the angular velocity

$$\text{(76)} \qquad |\nu_o| = |\nabla_s \phi_o|$$

of the rotation of the principal axis at the time $t = 0$ when the two eigenvalues of H_s coalesce.

In terms of the time $t = \ s$ as independent variable instead of s, formula (74) now reads

$$\text{(77)} \qquad \mathrm{Pr}_{\text{non-ad}} = \frac{2\pi}{|\nabla_t h_o|} |\nabla_t \phi_o|^2 .$$

Here we mean by $\nabla_t f_o$ the value of $\nabla_t f(t)$ for $t = 0$.

It is interesting to note that the probability that the process is nonadiabatic depends on the rate of change of the eigenvalues of the Hamiltonian at the angular velocity of the rotating principal axes only at the time when the two eigenvalues coalesce and that it becomes large when the two eigenvalues approach each other slowly while the principal axes rotate rapidly.

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